

10/S82,609
~~10/513699~~

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAEAL1624

PASSWORD:917P742

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CASREACT' AT 18:01:31 ON 13 AUG 2007
FILE 'CASREACT' ENTERED AT 18:01:31 ON 13 AUG 2007
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
ENTER STRUCTURE FORMAT (SIM), NOS:ide
'IDE' IS NOT A VALID STRUCTURE FORMAT KEYWORD
Structure Formats
SIA ----- Structure Image, Attributes, and map table if it contains
 data. (Default)
SIM ----- Structure Image.
SAT ----- Structure Attributes and map table if it contains data.
SCT ----- Structure Connection Table and map table if it contains
 data.
SDA ----- All Structure Data (image, attributes, connection table and
 map table if it contains data).
NOS ----- NO Structure data.
ENTER STRUCTURE FORMAT (SIM), NOS:end

=> .

. IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> file casreact

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 234.75 | 938.13 |

FILE 'CASREACT' ENTERED AT 18:05:20 ON 13 AUG 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
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Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 11 Aug 2007 VOL 147 ISS 8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*
* CASREACT now has more than 12 million reactions *
*

<12/04/2007>

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EAST Search History

| Ref # | Hits | Search Query | DBs | Default Operator | Plurals | Time Stamp |
|-------|------|---|-----------------|------------------|---------|------------------|
| L1 | 501 | (546/121,546/83,544/333,544/127). CCLS. | US-PGPUB; USPAT | OR | OFF | 2007/08/13 17:19 |
| L2 | 1 | L1 AND DIHYDROPYRANO | US-PGPUB; USPAT | OR | ON | 2007/08/13 17:20 |
| L3 | 1 | L2 AND IMIDAZO | US-PGPUB; USPAT | OR | ON | 2007/08/13 17:20 |
| L4 | 1 | L3 AND PYRIDINE | US-PGPUB; USPAT | OR | ON | 2007/08/13 17:20 |

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Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

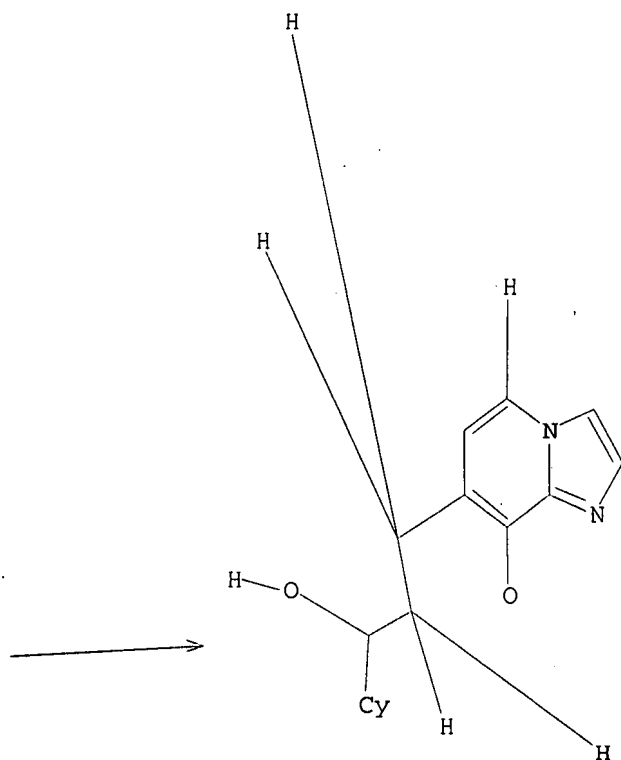
Uploading C:\Program Files\Stnexp\Queries\10582609b.str

L17 STRUCTURE UPLOADED

=> d l17

L17 HAS NO ANSWERS

L17 STR



Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\Program Files\Stnexp\Queries\10582609a.str

L18 STRUCTURE UPLOADED

=> d l18

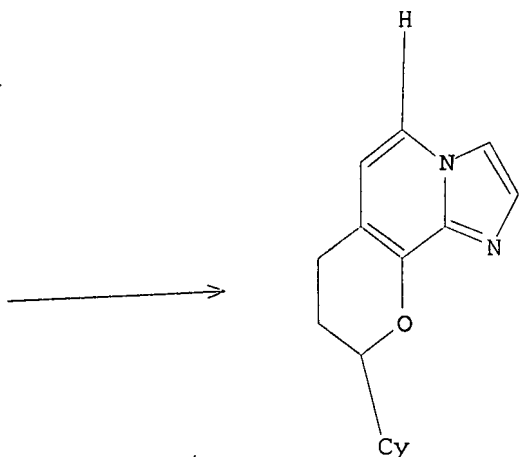
L18 HAS NO ANSWERS

L18 STR

<12/04/2007>

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Structure attributes must be viewed using STN Express query preparation.

=> s l17 full

FULL SEARCH INITIATED 18:06:08 FILE 'CASREACT'

SCREENING COMPLETE - 46 REACTIONS TO VERIFY FROM 6 DOCUMENTS

100.0% DONE 46 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

L19 0 SEA SSS FUL L17 (0 REACTIONS)

=> s l18 full

FULL SEARCH INITIATED 18:06:13 FILE 'CASREACT'

SCREENING COMPLETE - 1191 REACTIONS TO VERIFY FROM 57 DOCUMENTS

100.0% DONE 1191 VERIFIED 10 HIT RXNS 2 DOCS

SEARCH TIME: 00.00.01

L20 2 SEA SSS FUL L18 (10 REACTIONS)

=> d ibib abs fhit

L20 ANSWER 1 OF 2 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 111:77237 CASREACT

TITLE: Antiulcer agents. 4. Conformational considerations and the antiulcer activity of substituted imidazo[1,2-a]pyridines and related analogs

AUTHOR(S): Kaminski, James J.; Puchalski, Chester; Solomon, Daniel M.; Rizvi, Razia K.; Conn, David J.; Elliott, Arthur J.; Lovey, Raymond G.; Guzik, Henry; Chiu, P. J. S.; et al.

CORPORATE SOURCE: Pharm. Res. Div., Schering Res., Bloomfield, NJ, 07003, USA

SOURCE: Journal of Medicinal Chemistry (1989), 32(8), 1686-700
CODEN: JMCMAR; ISSN: 0022-2623

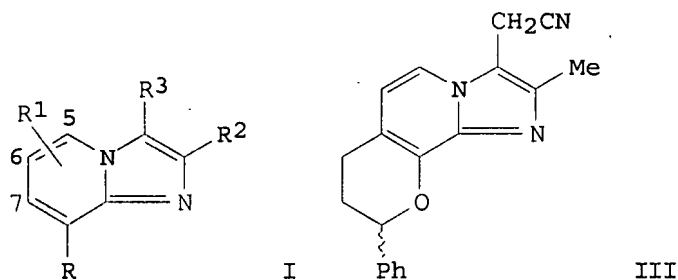
DOCUMENT TYPE: Journal

LANGUAGE: English

GI

<12/04/2007>

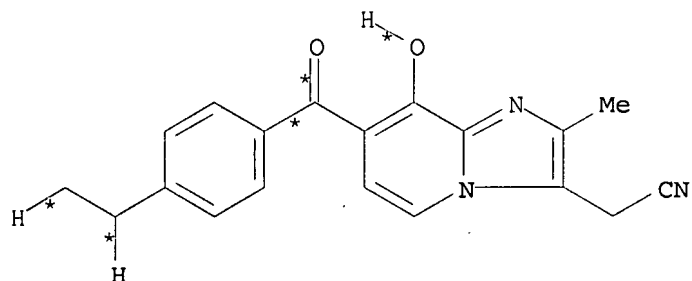
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AB Definition of the interrelationship between the conformational characteristics of a series of substituted imidazo[1,2-a]pyridines and their antiulcer activity was investigated by examining the conformational properties of imidazo[1,2-a]pyridine I [R = PhCH₂O, R₁ = H, R₂ = Me, R₃ = CH₂CN (II)], by using a variety of exptl. and theor. methods. The result of these studies was the identification of two distinctly different candidates, designated the folded and the extended conformation, resp., to represent the two possible min.-energy conformations of II. In order to select the biol. relevant conformer, a group of 3-substituted 2-methylimidazo[1,2-a]pyridines, having either a cis- or a trans-2-phenylethenyl substituent at the 8-position, were designed as conceptually simple and synthetically accessible semirigid analogs of the resp. candidate conformers. Gastric antisecretory activity was found to reside only in the trans isomers I (R = trans-PhCH:CH, R₁ = H, R₂ = Me; R₃ = Me, CH₂CN, NH₂), which mimic the extended conformation. This observation led to the construction of imidazo[1,2-a]pyrano[2,3-c]pyridine-3-acetonitrile (III), a rigid tricyclic analog that is effectively locked in the extended conformation and that exhibited an antiulcer profile comparable to that of prototype II. These results unequivocally demonstrate that, in accord with expectation for a drug operating at a specific receptor, the conformational characteristics of the mol. have a substantial effect in determining its antiulcer activity. More precisely, it has been demonstrated that it is the extended conformation of II that represents the bioactive form of the drug. These results constitute the basis for a mol. probe that should aid in the investigation of the as yet uncharacterized gastric proton pump enzyme (H⁺/K⁺-ATPase), by means of which II and its analogs presumably exert their pharmacol. actions.

RX(54) OF 213 ...DT ==> DU...

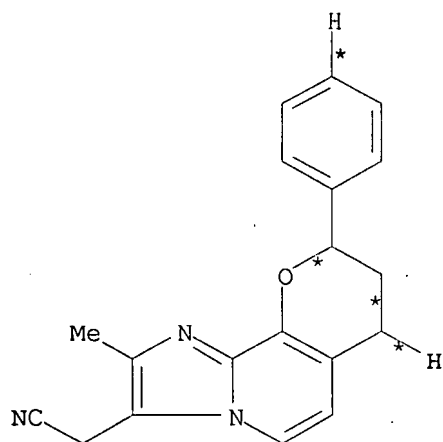
10/513699



● HCl

DT

(54) →



DU

RX(54) RCT DT 121394-50-1

STAGE(1)

RGT C 16940-66-2 NaBH4

SOL 64-17-5 EtOH, 75-09-2 CH2Cl2

STAGE(2)

RGT DV 109-63-7 BF3-Et2O

SOL 75-09-2 CH2Cl2

PRO DU 93749-57-6

NTE sand used in second step

=> d ibib abs hitstr 2

'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

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ABS ----- GI and AB
 ALL ----- BIB, AB, IND, RE, Single-step Reactions
 APPS ----- AI, PRAI
 BIB ----- AN, plus Bibliographic Data
 CAN ----- List of CA abstract numbers without answer numbers
 CBIB ----- AN, plus Compressed Bibliographic Data
 DALL ----- ALL, delimited (end of each field identified)
 IABS ----- ABS, indented with text labels
 IALL ----- ALL, indented with text labels
 IBIB ----- BIB, indented with text labels
 IND ----- Indexing data
 IPC ----- International Patent Classifications
 ISTD ----- STD, indented with text labels
 OBIB ----- AN, plus Bibliographic Data (original)
 OIBIB ----- OBIB, indented with text labels

 SBIB ----- BIB, no citations
 SIBIB ----- IBIB, no citations

 MAX ----- Same as ALL
 PATS ----- PI, SO
 SCAN ----- TI and FCRD (random display, no answer number. SCAN
 must be entered on the same line as DISPLAY, e.g.,
 D SCAN.)
 SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for
 all single-step reactions)
 STD ----- BIB, IPC, and NCL

 CRD ----- Compact Display of All Hit Reactions
 CRDREF ----- Compact Reaction Display and SO, PY for Reference
 FHIT ----- Reaction Map, Diagram, and Summary for first
 hit reaction
 FHITCBIB --- FHIT, AN plus CBIB
 FCRD ----- First hit in Compact Reaction Display (CRD) format
 FCRDREF ----- First hit in Compact Reaction Display (CRD) format with
 CA reference information (SO, PY). (Default)
 FPATH ----- PATH, plus Reaction Summary for the "long path"
 FSPATH ----- SPATH, plus Reaction Summary for the "short path"
 HIT ----- Reaction Map, Reaction Diagram, and Reaction
 Summary for all hit reactions and fields containing
 hit terms
 OCC ----- All hit fields and the number of occurrences of the
 hit terms in each field. Includes total number of
 HIT, PATH, SPATH reactions. Labels reactions that have
 incomplete verifications.
 PATH ----- Reaction Map and Reaction Diagram for the "long
 path". Displays all hit reactions, except those
 whose steps are totally included within another hit
 reaction which is displayed
 RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)
 RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)
 RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
 RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)
 SPATH ----- Reaction Map and Reaction Diagram for the "short
 path". Displays all single step reactions which
 contain a hit substance. Also displays those
 multistep reactions that have a hit substance in both
 the first and last steps of the reaction, except for

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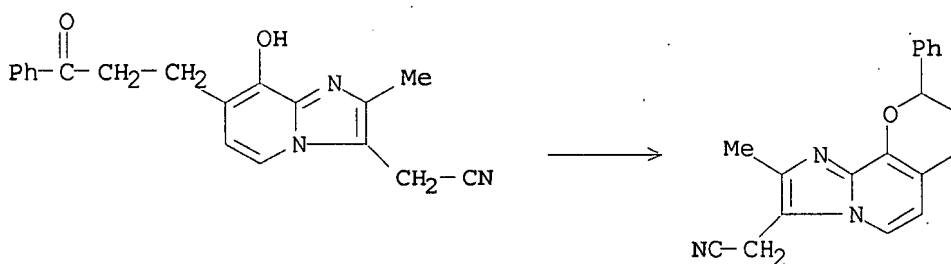
those hit reactions whose steps are totally included
within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):.

L20 ANSWER 2 OF 2 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 3



HCl

REF: U.S., 4468400, 28 Aug 1984

=> d his

(FILE 'HOME' ENTERED AT 17:27:32 ON 13 AUG 2007)

FILE 'REGISTRY' ENTERED AT 17:27:41 ON 13 AUG 2007

L1 STRUCTURE UPLOADED

L2 189 S L1 FULL

FILE 'CAPLUS' ENTERED AT 17:28:17 ON 13 AUG 2007

L3 25 S L2 FULL

FILE 'REGISTRY' ENTERED AT 17:30:26 ON 13 AUG 2007

L4 STRUCTURE UPLOADED

L5 189 S L1 FULL

L6 20 S L4 FULL

L7 11 S L1

L8 1 S L4

FILE 'REGISTRY' ENTERED AT 17:42:10 ON 13 AUG 2007

L9 STRUCTURE UPLOADED

L10 189 S L9 FULL

FILE 'CAPLUS' ENTERED AT 17:42:34 ON 13 AUG 2007

L11 25 S L10 FULL

FILE 'CASREACT' ENTERED AT 17:46:49 ON 13 AUG 2007

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| | |
|-----|--------------------|
| L12 | STRUCTURE UPLOADED |
| L13 | STRUCTURE UPLOADED |
| L14 | 0 S L12 |
| L15 | 2 S L12 FULL |
| L16 | 0 S L13 FULL |

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| | |
|-----|--------------------|
| L17 | STRUCTURE UPLOADED |
| L18 | STRUCTURE UPLOADED |
| L19 | 0 S L17 FULL |
| L20 | 2 S L18 FULL |